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## Noise Propagation and Uncertainty Quantification in Hybrid Multiphysics Models

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Final Report

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**Task:** Initiation and Reaction Propagation in Energetic Materials

**AFOSR award:** FA9550-12-1-0185

**Program Manager:** Dr. Jennifer L. Jordan, Dynamic Materials and Interactions Program

**PI:** Prof. Daniel M. Tartakovsky, University of California, San Diego

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The following manuscripts have been co-authored by the members of our research team (D. M. Tartakovsky, J. Bakarji, K. Zamani, A. Pigarov) with financial support from AFOSR.

1. Bakarji, J. and D. M. Tartakovsky, On the use of reverse Brownian motion to accelerate hybrid simulations, *J. Comput. Phys.* (under review, JCOMP-D-16-00742), 2016.
2. Taverniers, S. and D. M. Tartakovsky, A tightly-coupled domain-decomposition approach for nonlinear stochastic multiphysics systems, *J. Comput. Phys.* (under review, JCOMP-D-16-00398), 2016.
3. Dentz, M., I. Neuweiler, Y. Méheust, and D. M. Tartakovsky, Noise-driven interfaces and their macroscopic representations, *Phys. Rev. E* (under review, LH14939), 2016.
4. Boso, F. and D. M. Tartakovsky, The method of distributions for dispersive transport in porous media with uncertain properties, *Water Resour. Res.* (in press, 2016WR018745R) 2016.
5. Taverniers, S., A. Y. Pigarov, and D. M. Tartakovsky, Conservative tightly-coupled simulations of randomly fluctuating multiscale systems, *J. Comput. Phys.*, 313, 400-414, doi:10.1016/j.jcp.2016.02.047, 2016.
6. Barajas-Solano, D. A. and D. M. Tartakovsky, Stochastic collocation methods for non-linear parabolic equations with uncertain parameters, *SIAM/ASA J. Uncert. Quant.*, 4(1), 475-494, doi:10.1137/130930108, 2016.
7. Ruiz-Martinez, A., T. M. Bartol, T. J. Sejnowski, and D. M. Tartakovsky, Efficient multiscale models of polymer assembly, *Biophys. J.*, doi:10.1016/j.bpj.2016.05.022, 2016.

8. Sinsbeck, M. and D. M. Tartakovsky, Impact of data assimilation on cost-accuracy tradeoff in multifidelity models, *SIAM/ASA J. Uncert. Quant.*, 3(1), 954-968, 2015.
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11. Barajas-Solano, D. A., B. E. Wohlberg, V. V. Vesselinov, and D. M. Tartakovsky, Linear functional minimization for inverse modeling, *Water Resour. Res.*, 51, doi:10.1002/2014WR016179, 2015.
12. Regner, B. M., D. M. Tartakovsky and T. J. Sejnowski, Identifying transport behavior of single-molecule trajectories, *Biophys. J.*, 107(10), 2345-2351, 2014.
13. Boso, F., S. V. Broyda, and D. M. Tartakovsky, CDF solutions of advection-reaction equations with uncertain parameters, *Proc. R. Soc. A*, 470(2166), 20140189, 2014.
14. Taverniers, S., F. J. Alexander, and D. M. Tartakovsky, Noise propagation in hybrid models of nonlinear systems: The Ginzburg-Landau equation, *J. Comput. Phys.*, 262, 313-324, 2014.

## 2 Technical accomplishments

Granular energetic materials exhibit complex chaotic behavior due to the coexistence of a wide range of energy scales without scale separation. The main challenges involved in modeling the physical processes leading to initiation of explosive reactions are (i) the lack of a general model for heterogeneous granular media under compaction and (ii) the lack of a reliable multi-scale discrete-to-continuum framework for describing diffusion-advection-reaction processes in complex particulate media. Most conventional methods for studying viscoplastic deformations of granular media under shear and compression in ideal conditions overlook the effect of spatial heterogeneity in granular structure. This heterogeneity is believed to play a major role in stress and heat localization events responsible for initiating reactions in energetic materials. In particular, it has been observed that so-called “hot-spots” emerge as a consequence of visco-plastic pore collapse, inter-granular friction, and granular compaction. The wide range in stress,

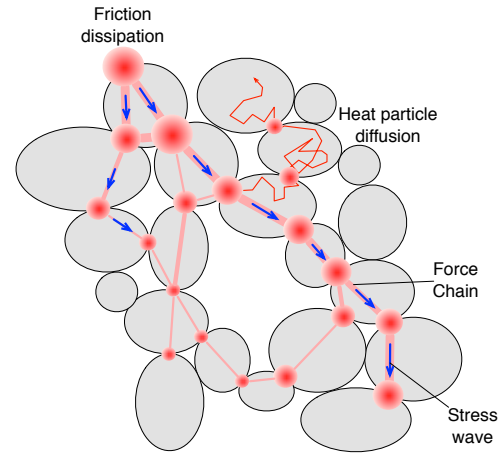


Figure 1: Interaction between granular dissipation due to friction, stress waves and heat diffusion.

strain, and dissipation found in energetic materials magnify the multiscale behavior of the system. That is, microscopic events invariably affect the macroscopic behavior of the system and cannot be neglected, yet are also impossible to predict deterministically. Specifically, macroscopic stress boundary conditions induce heterogeneous deformations at the grain level which causes friction and grain deformations at the microscopic level. This generates thermal fluctuations and chemical reactions at the molecular level, which in turn builds up a shock wave whose power is several orders of magnitude higher than the initial conditions.

During the two years of this project we investigated two of the processes in Figure 1: multiscale diffusion / heat transfer and multiscale dynamics of granular materials.

## 2.1 Hybrid Discrete-Continuum Models of Heat Dissipation

Efficient coupling of continuum (deterministic or stochastic) constitutive solvers with their discrete (stochastic, particle-based) counterparts is a common challenge in hybrid and multiphysics simulations. We [Bakarji and Tartakovsky, 2016] studied interfacial, tightly coupled simulations of diffusion that combine continuum and particle-based solvers. The latter employed the reverse Brownian motion (rBm), a Monte Carlo approach that allows one to enforce inhomogeneous Dirichlet, Neumann, or Robin boundary conditions and is trivially parallelizable. In Brownian motion, a particle's trajectory  $\mathbf{X}(t)$  evolves in time according to a stochastic differential equation  $d\mathbf{X}(t) = \sqrt{2\alpha_d} d\mathbf{W}(t)$  where  $\alpha_d$  is a diffusion coefficient, and  $d\mathbf{W}(t) \sim \mathcal{N}(0, dt)$  is a  $d$ -dimensional Wiener process. Our Monte Carlo simulations used the rBm implementation, in which individual trajectories of  $N_{\text{MC}}$  particles released at point  $\mathbf{x}$  at time  $t$  satisfy  $\mathbf{X}(t - \Delta t_d) = \mathbf{X}(t) - \sqrt{2\alpha_d} \mathcal{N}(0, \Delta t_d)$ . Given an initial condition  $u_{\text{in}}(\mathbf{x})$ , and the functions  $u_{\text{D}}(\mathbf{x}, t)$  and  $J_{\text{N}}(\mathbf{x}, t)$  prescribed respectively on the Dirichlet and Neumann boundary conditions, the sample mean temperature  $\hat{u}_d(\mathbf{x}, t)$  at space-time point  $(\mathbf{x}, t)$  is computed as a weighted sum

$$\hat{u}_d(\mathbf{x}, t) = \frac{N_{\text{in}}}{N_{\text{MC}}} \mathcal{S}_{\text{in}} + \frac{N_{\text{D}}}{N_{\text{MC}}} \mathcal{S}_{\text{D}} + \frac{N_{\text{N}}}{N_{\text{MC}}} \mathcal{S}_{\text{N}} \quad (1)$$

of sample averages of the initial and boundary functions,  $u_{\text{in}}[\mathbf{X}_i(0)]$ ,  $u_{\text{D}}[\mathbf{X}_i(t - T_i), t - T_i]$  and  $J_{\text{N}}[\mathbf{X}_i(t - T_{i,j}), t - T_{i,j}]$ . Here  $N_{\text{in}}$ ,  $N_{\text{D}}$  and  $N_{\text{N}}$  are the numbers of particles that reached the initial state and the boundaries, respectively; and  $T_i$  is the  $i$ th particle's exit time.

We developed a number of numerical approaches for improving the accuracy of rBm in the presence of inhomogeneous Neumann boundary condition and alternative strategies for coupling the rBm solver with its continuum counterpart. Numerical experiments were used to investigate the convergence, stability, and computational efficiency of the proposed hybrid algorithm. Our analysis revealed that the use of Monte Carlo simulations based on the reverse Brownian motion (rBm) in the context of discrete-to-continuum hybrid simulations has a number of advantages. These include

1. the ability to use very large hybrid time step  $\Delta t_{\text{h}}$  without compromising accuracy,
2. the ability to compute the solution only near the boundaries to ensure the continuity of the flux in the hybrid method,

3. the ability to use the continuum domain as a deterministic source of Dirichlet, Neumann and initial boundary conditions for the rBm, and therefore
4. a controllable loss of accuracy given a flexible choice of  $N_{MC}$  at every location in the particle domain.

Our hybrid algorithm is easy to implement in any number of dimensions. Furthermore, extending the hybrid model to advection-diffusion equations is relatively straightforward.

## 2.2 Hybrid Discrete-Continuum Models of Compaction of Granular Materials

Given a force applied to the top of a cylinder filled with monodisperse granular medium with spherical metal beads (Figure 2), find the height of the top lid  $h(t)$  as a function of time. The particles are assumed to be formed of a deformable and incompressible metal (e.g., aluminum). The pressure  $P$  on the top is assumed to be constant. It is expected that the presence of a large pore will induce more compactions, i.e.,  $h_{\text{pore}} < h_{\text{hom}}$ . We estimated the height of the lid in the presence of a macro-pore as compared to the case without macro-pores. More specifically, we studied the effects of heterogeneity by using a local model for pore collapse in a granular medium.

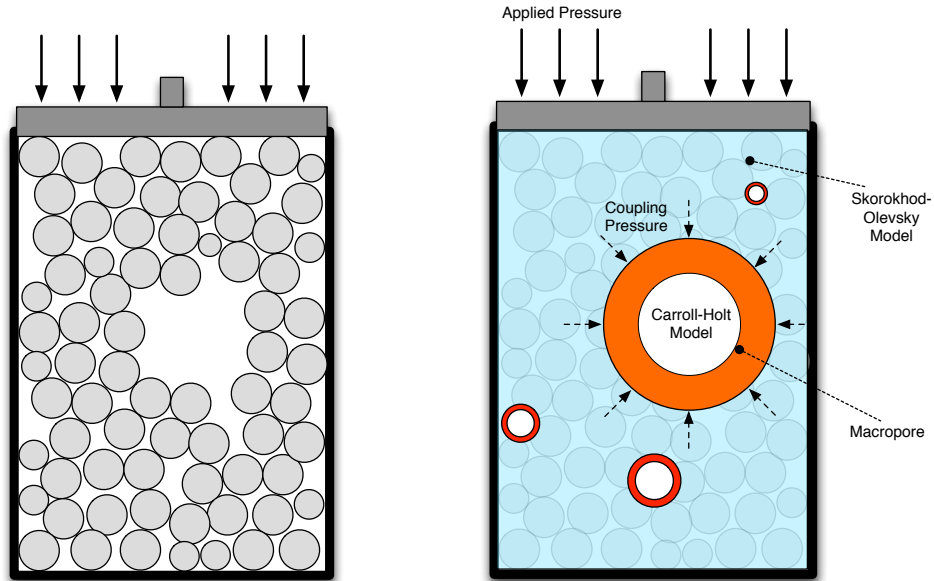


Figure 2: A physical system (left) and its hybrid model (right).

A discrete representation of a granular material's dynamics was based on the Carroll-Holt (CH) model, which is an axisymmetric elasto-plastic model of the collapse of an incompressible metallic shell. We used the modified CH model that introduces a restriction on the extent to which the pore can collapse, avoiding singularity at its center. While using this model, the coupling has to be done in a way that transforms the compressible shell of the actual case into an incompressible shell.





stress distribution around the pores can be deduced by assuming the pores to be in an infinite medium (compared to the whole domain). Figure 4a shows the combined effect of multiple macropores using a superposition of Carroll-Holt models with different radii and surface stresses. This gives an idea on what to expect in the difference between a homogeneous and heterogeneous compaction.

Assuming a linear-viscous continuum model for the matrix, we explored the dependence of the height of the lid  $h(t)$  as a function of viscosity. Figure 4b shows a range of viscosity of one order of magnitude.

## 2.3 Fluctuating Macroscopic Models

Inspired by fluctuating Navier-Stokes equations of hydrodynamics, we explored ways to model unresolved micro-scales, e.g., heterogeneity due to macropores, as a random source in the Cauchy equation of motion,

$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \mathcal{I}_p \mathbf{f}(\mathbf{x}, t) \quad (4)$$

where  $\rho$  is the density,  $\mathbf{u}$  is the velocity at point  $\mathbf{x}$  and time  $t$ , and the stress tensor  $\boldsymbol{\sigma}$  is related to the strain rate  $\dot{\epsilon}$  by a constitutive law, e.g., by the Skorokhod-Olevsky relation (2). The (possibly random) indicator function  $\mathcal{I}_p(\mathbf{x})$  for a macropore region  $\Omega_p(t)$  is defined as  $\mathcal{I}_p = 1$  if  $\mathbf{x} \in \Omega_p$  and  $= 0$  otherwise. The macropore region  $\Omega_p(t)$  is a multi-connected domain comprising multiple macropores, which can be randomly distributed throughout the material. The random source vector  $\mathbf{f}(\mathbf{x}, t)$  is treated as zero-mean white noise,  $\mathbb{E}[\mathbf{f}(\mathbf{x}, t)] = \mathbf{0}$ ,  $\mathbb{E}[f_i(\mathbf{x}, t) f_j(\mathbf{y}, \tau)] = v_i^2 \delta(\mathbf{x} - \mathbf{y}) \delta(t - \tau)$  where  $v_i^2$  is the variance of the  $i$ th component of the noise and  $\delta(\cdot)$  is the Dirac delta function. Figure 5 exhibits an average velocity distribution within the granular material undergoing slow compaction, for the case of a single macropore and given noise strength  $v_i^2$ .

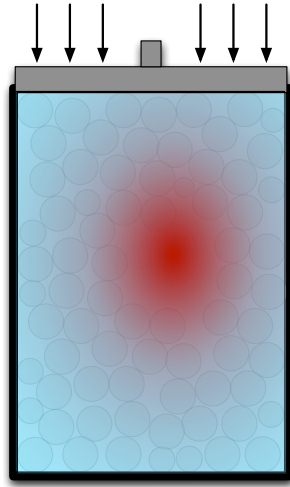


Figure 5: Average velocity distribution within the granular material undergoing compaction.

Our still elusive goal is to relate the variance  $v_i^2$  to material properties, e.g., grain-size distribution, via the fluctuation-dissipation theorem.

1.

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**Abstract**

Granular energetic materials exhibit complex chaotic behavior due to the coexistence of a wide range of energy scales without scale separation. The main challenges involved in modeling the physical processes leading to initiation of explosive reactions are (i) the lack of a general model for heterogeneous granular media under compaction and (ii) the lack of a reliable multiscale discrete-to-continuum framework for describing diffusion-advection-reaction processes in heterogeneous particulate media. This heterogeneity plays a major role in stress and heat localization, which is responsible for initiating reactions in energetic materials. In particular, hot-spots emerge as a consequence of visco-plastic pore collapse, inter-granular friction, and granular compaction. We developed a number of computation tools for stochastic analysis of granular materials dynamics. These include a continuum-discrete model of heat dissipation/diffusion and a continuum-discrete model of compaction of a granular material with macro-pores. We have also proposed a class of randomly fluctuating macroscopic equations of motion for granular materials and powders.

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